Entanglement entropy of a quantum unbinding transition and entropy of DNA

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Abstract –Two significant consequences of quantum fluctuations are entanglement and critical-ity. Entangled states may not be critical but a critical state shows signatures of universality in entanglement. A surprising result found here is that the entanglement entropy may become arbi-trarily large and negative near the dissociation of a bound pair of quantum particles. Although apparently counter-intuitive, it is shown to be consistent and essential for the phase transition, by mapping to a classical problem of DNA melting. We associate the entanglement entropy to a subextensive part of the entropy of DNA bubbles, which is responsible for melting. The absence of any extensivity requirement in time makes this negative entropy an inevitable consequence of quantum mechanics in continuum. Our results encompass quantum critical points and first-order transitions in general dimensions.

Introduction. – Quantum entanglement [1–4] is a fundamental feature of quantum mechanics, which says that performing a local measurement may instantaneously affect the outcome of local measurements far away. There is another feature of quantum mechanics where the zero-point fluctuations in the ground state may coherently add up to produce long-range correlations of local observables. This happens at quantum critical points (QCP), a point where the spectrum becomes gapless, obtained by tun-ing the parameters of the Hamiltonian. In both cases, a pure state cannot be written as the product of the wave-functions of the two distant parts, though states may be entangled without being critical. The ground-state energy may be non-analytic through a quantum phase transition (QPT) or through a quantum critical point. The wave function encodes not only this non-analyticity but also the special quantum correlations or quantum entanglement in-trinsic to the state.

At or near a QCP, the signatures of its universality can therefore be found in the entanglement, a common mea-sure of which is the von Neumann entropy (S) [3–8]. The exact results of this paper show that for a class of critical points, viz., the dissociation of a pair of particles in the unitarity limit of infinite scattering length, there is the possibility of a negatively diverging S. Although counter-intuitive, this is not an artifact. Analogous situation oc-curs in statistical mechanics for Gibbs entropy in canoni-cal ensemble for a gapless spectrum. As discussed below, the problem in hand involves a gapless entanglement spec-trum. The usual proof of the positivity of entanglement entropy is not applicable in case of continuous eigenvalues of the reduced density matrix. The negative entropy is es-sential for the criticality itself. Its importance is brought out via the mapping of the quantum problem to the equiv-alent classical statistical mechanical problem, the melting of a double-stranded DNA [9–12].

Entanglement entropy. – Recall the problem of a quantum particle of mass m in a three dimensional spher-ical potential well,

$$V(\mathbf{r}) \quad = \quad -V_0 \qquad \text{for } r < a,$$
$$= \quad 0 \qquad \text{for } r > a, \qquad (1)$$

where r is the radial coordinate, a and V_0 are the width and the depth of the potential well. What is special is that $V_0 > 0$ does not guarantee the existence of a bound state, unlike in one or two dimensions, or in classical mechanics. No bound state exists for $u < u_c$ where $u = 2mV_0a^2/\hbar^2$ is the dimensionless parameter for the potential and u_c cor-responds to a critical value of u. For simplicity, we take $u \approx u_c$ so that there is only one bound state. In this situa-tion energy $|E|$ itself is the gap in the spectrum. If we tune u to get a state with zero energy $(E = 0)$, then at that energy in $d = 3$ the wave function $\varphi(r) \sim 1/r$ which is like a non-normalizable critical state. Like a bound state the
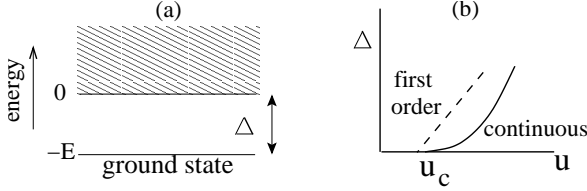
Fig. 1: (a) Gap Δ in the energy spectrum. The shaded region is the continuum of energy. (b) The graph shows how energy gap goes to zero. The continuous line describes a second order or continuous transition (critical) and the dashed line shows the first order transition. The two are distinguished by the behaviour of the slope at $u = u_c$.

Fig. 2: Path integral representation in the x-t plane. (a) A relative coordinate path for two particles in one-dimension. The solid portions represent the classical bound state, i.e., inside the well (B), and the dashed portions represent the unbound (U) state in the classically forbidden region. (b) Corresponding path representation of two quantum particles with time, though intersections of paths are not shown explicitly. It is also a configuration of two classical Gaussian polymers interacting at the same contour length as for DNA base pairing, the t-axis representing the contour length (z) of the polymers. The dotted lines are the melted bubbles whose partition functions are characterized by the reunion exponent Ψ. This description holds for any general d.

probability density does decay to zero but like an unbound state it is not normalizable. In higher dimensions, the condition for a minimal strength of the potential for a bound state remains true, but the state corresponding to $E = 0$ becomes normalizable as it should be for a bound state. So we see that this bound to unbound transition for a potential well has different nature in different dimensions. In general, (i) for $d \leq 2$ there is no such transition as $E = 0$ requires $V_0 = 0$, though there are remnants of the transition as $V_0 \to 0$, (ii) for $2 < d < 4$, the transition is continuous (critical) — the bound state becomes unbound through a non-normalizable critical state as we change u, and, (iii) for $d > 4$, the bound state remains normalizable up to and including $E = 0$, and becomes unbound as u is decreased further, thus making the transition first-order. This depicts a QPT and the case of a potential well gives a simple example of a quantum critical point for $2 < d < 4$ with diverging length scales.

The ground state energy, for u close to u_c, is the gap Δ in the spectrum. A quantum phase transition is characterized by a vanishing gap. A discontinuity of the first derivative $d\Delta/du$ signals a first order transition, otherwise it is critical or continuous, as shown in Fig. 1. One may define characteristic time and length scales

$$\xi_\parallel = \hbar\Delta^{-1}, \text{ and } \xi_\perp = \hbar/\sqrt{2m\Delta}, \qquad (2)$$

both of which diverge as $\Delta \to 0$, with $\xi_\parallel \sim \xi_\perp^z$, $z (= 2$ in this case) being the dynamic exponent. One may compare with the classical ground state to see the importance of quantum (zero-point) fluctuations and the importance of time or dynamics in quantum phase transitions. A path-integral interpretation of these scales, useful for the DNA mapping, is given below.

Let us now consider the ground state of two dissimilar particles interacting via a central potential $V(|\mathbf{r}_1 - \mathbf{r}_2|)$ of the type of Eq. 1, with $\mathbf{r}_i$ denoting the co-ordinate of the i-th particle. The existence of diverging length scales and scaling behavior around $u = u_c$ justifies the dissociation of the bound pair to be a QCP or a QPT depending on the dimensions they are in. The criticality is described by the exponents for the diverging length scales and the energy,
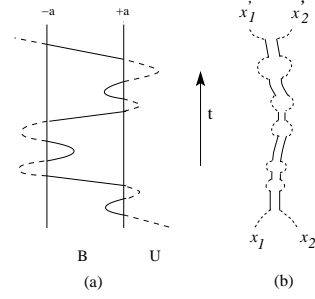
as

$$|E| \sim \xi_\parallel^{-1} \sim |u - u_c|^{\nu_\parallel}, \text{ and } \xi_\perp \sim |u - u_c|^{-\nu_\perp}, \qquad (3)$$

with

$$\nu_\parallel = z\nu_\perp = 1/(\Psi - 1), \text{ for } 1 < \Psi \leq 2, \qquad (4)$$
$$= 1, \qquad \text{for } \Psi \geq 2, \qquad (5)$$

which involve (i) z the dynamic exponent, and (ii) a universal exponent Ψ, known as the reunion exponent for polymers [9–11]. For the short range interaction problem, $\Psi = d/2$, as for random walkers, from which the specialty of $d = 4$ is apparent.

In a quantum bound state a particle can tunnel through the potential. In a path integral approach the particle does a sizable excursion in the classically forbidden region outside the interaction well, sooner or later returning to the well (see Fig. 2). That the two particles will eventually be close-by to form a bound state is the source of entanglement while the excursions produce spreads of the trajectories in space and time. These spreads give the two relevant length scales $\xi_\parallel, \xi_\perp$. The large width of the bound state wave function near the QCP ensures the mutual influence of the particles even if far away from each other ($r \gg a$) so that the reduced density matrix for one particle still carries the signature of the entanglement and the criticality. For this bipartite system, we are interested in the "particle-partitioning entanglement" [13]. This makes the von Neumann entropy a valuable quantity for the transition which reads,

$$S = -\text{Tr } \rho \ln \rho, \qquad (6)$$

where ρ is the reduced density matrix for the ground state $|\psi\rangle$,

$$\rho(\mathbf{r}_1, \mathbf{r}'_1) = \mathrm{Tr}_2 \ \varrho(1,2) = \int d^d\mathbf{r}_2 \ \langle \mathbf{r}_1, \mathbf{r}_2 | \psi \rangle \langle \psi | \mathbf{r}'_1, \mathbf{r}_2 \rangle, \quad (7)$$

obtained from the two particle density matrix $\varrho(1,2) = |\psi\rangle\langle\psi|$ by integrating out (or tracing out) particle 2. In Eq. 6, we shall introduce some pre-chosen length scale to make the argument of log dimensionless. If, with $m_i, \mathbf{r}_i$ denoting the mass and the position of the ith particle, the full ground state wave-function (including the center of mass (CM)) is

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \Phi\left(\frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}\right) \varphi(\mathbf{r}_1 - \mathbf{r}_2), \qquad (8)$$

where Φ is CM wave function (plane waves) and φ is the wave function in relative coordinate (the relative wave-function), then

$$\rho(\mathbf{r}_1, \mathbf{r}'_1) = \int d^d\mathbf{r}_2 \ \psi(\mathbf{r}_1, \mathbf{r}_2)\psi^*(\mathbf{r}'_1, \mathbf{r}_2). \qquad (9)$$

Although the center of mass and the relative parts are not entangled, the two particles are entangled. The lack of knowledge of the state of one particle is the source of a nonzero entropy associated with the reduced density matrix [1–3].

The translational invariance of the interaction guarantees that the reduced density matrix $\rho(\mathbf{r}, \mathbf{r}') \equiv \rho(\mathbf{r} - \mathbf{r}')$ has $\exp(-i\mathbf{q}\cdot\mathbf{r})$ as the eigenvector,

$$\int d^d\mathbf{r}' \rho(\mathbf{r} - \mathbf{r}')e^{-i\mathbf{q}\cdot\mathbf{r}'} = \hat{\rho}(\mathbf{q}) \, e^{-i\mathbf{q}\cdot\mathbf{r}}, \qquad (10)$$

with the eigenvalue

$$\hat{\rho}(\mathbf{q}) = \left|\phi\left(\mathbf{q} + \frac{\mathbf{K}\mu}{m_2}\right)\right|^2, \qquad (11)$$

$\mathbf{K}$ being CM wave vector and $\phi(\mathbf{q})$ the normalized momentum space wave function, the Fourier transform of the relative wave-function $\varphi(\mathbf{r})$ in Eq. 8. Since the entropy involves an integral over the whole range of $\mathbf{q}$, it is independent of the CM wave-vector, an expected consequence of Galilean invariance. Therefore, without any loss of generality, we choose $|\mathbf{K}| = 0$. The eigenvalues constituting the "entanglement spectrum" can be written in a scaling form

$$|\phi(\mathbf{q})|^2 = \kappa^{-d} \ F(\mathbf{q}/\kappa, a\kappa), \qquad (12)$$

where $\kappa^2 = 2\mu|E|/\hbar^2 = \xi_\perp^{-2}$, μ being the reduced mass. Eq. 12 satisfies $\mathrm{Tr}\ \hat{\rho} = 1$. In the critical regime (also called the "unitarity limit"), $a\kappa \to 0$, if the scaling function behaves smoothly, then

$$F(\tilde{\mathbf{q}}, a\kappa) \to F(\tilde{\mathbf{q}}, 0) \equiv f(\tilde{\mathbf{q}}), \quad (\tilde{q} \equiv q/\kappa) \qquad (13)$$

which we find to be true for $d < 4$. For $d \geq 4$, we find that $F(\tilde{\mathbf{q}}, a\kappa)$ for $a\kappa \to 0$ behaves in a singular fashion as

$$F(\mathbf{x}, y) \sim y^{d-4}f(\mathbf{x}), \qquad (14)$$

so that the prefactor in Eq. 12 becomes $\kappa^{-4}a^{d-4}$. Here f represents a generic function. By using these limiting forms, we find the entanglement entropy to be

$$S = P \ln a\kappa + c_0, \qquad (15a)$$
$$P = \min(d,4), \ \text{and} \quad c_0 = -\int d^dx \ f(x)\ln f(x). \qquad (15b)$$

The last statement can be verified by direct computation of the momentum distribution function of the relative motion in d-dimensions. There are further log-corrections at $d = 2$ and $d = 4$ which we do not discuss here.

To motivate Eq. 15a let us consider a few examples. Consider the quantum problem of two particles interacting via a delta-function potential in one dimension: $V(\mathbf{x}) = -v_0\delta(x)$. By using the center of mass and the relative coordinate wave-function, we write the wave function as

$$\psi(x_1, x_2) = C \ e^{iK\mu\left(\frac{x_1}{m_2} + \frac{x_2}{m_1}\right)} e^{-\kappa|x_1 - x_2|} \qquad (16)$$

which is translationally invariant. Here K is the CM wave vector, $\kappa = \xi_\perp^{-1}$, and C is the normalization constant. The reduced density matrix for particle 1 is then

$$\rho(x, x') = \frac{C^2}{\kappa} \ e^{-(iK\mu/m_2 + \kappa)|x' - x|} [1 + \kappa|x - x'|] \qquad (17)$$

having eigenvalues (Eq. 11)

$$\hat{\rho}(\mathbf{q}) = \frac{2}{\pi}\frac{1}{\kappa}\frac{1}{(1 + \tilde{q}^2)^2}, \ (K = 0), \qquad (18)$$

which is of the form Eq. 13 with $f(\tilde{\mathbf{q}}) \sim (1 + \tilde{q}^2)^{-2}$. By introducing an arbitrarily chosen well strength $\bar{v}$ or a scale $a = \hbar^2/2\mu\bar{v}$ in Eq. 6, the entanglement entropy is found to be of the form of Eq. 15a with

$$P = 1, \ \text{and} \ c_0 = \ln 8\pi - 2. \qquad (19)$$

For $\kappa \to 0$, $\hat{\rho}(\mathbf{q}) \to \delta(q)$ with $S = 0$. There is a difference between $\kappa \to 0$ and $\kappa = 0$.

For a one-dimensional problem with the potential of Eq. 1, one can go over to the delta function potential problem by taking $a \to 0$ keeping $V_0 a = v_0$ constant to get the same $\ln \kappa$ behaviour as in Eq. 19.

We then check for a 3-dimensional potential well, Eq. 1. The relative wave-function ($l = 0$) for this potential is

$$\varphi(\mathbf{r}) = \begin{cases} A \ \frac{\sin kr}{r} & r < a \\ B \ \frac{e^{-\kappa r}}{r} & r > a, \end{cases} \qquad (20)$$

with k and κ as defined earlier and constants A, B determined in the usual way of continuity of the wave function and its derivative. A direct Fourier transformation of $\varphi(\mathbf{r})$ has been used to numerically compute the entanglement entropy. To derive an analytical formula, we note that the dominant contribution in $\hat{\rho}(\mathbf{q})$ in the limit $a\kappa \to 0$ comes from the outer part. In this approximation we get

$$\hat{\rho}(\mathbf{q}) = \frac{1}{\kappa^3}\frac{1}{\pi^2}\left(\frac{1}{1 + \tilde{q}^2}\right)^2 = \kappa^{-3}f(\tilde{\mathbf{q}}). \qquad (21)$$

This $\hat{\rho}(\mathbf{q})$ satisfies the normalization condition $\int d^3q \ \hat{\rho}(\mathbf{q}) = 1$. Thus for the 3D potential well interaction, the entanglement entropy is of the form of Eq. 15a with

$$P = 3, \text{ and } c_0 = 2(1 + \log(4\pi)) \approx 7.06205. \tag{22}$$

Exact numerical computations of von Neumann entropy for $d = 3$ are done by using MATHEMATICA. For a given κ with $a = 1$, we determine V_0, the depth of the well and then the matching conditions and the Fourier transform were used to obtain the entanglement spectra. The entanglement entropy is then obtained by a numerical integration. The results are shown in a log-linear S vs. κ plot in Fig 3 which also shows the line obtained from Eq. 15a and Eq.22. It shows that S is negative for small κ and that it has linear $\ln \kappa$ dependence. The approximations show that the entropy is determined mainly by the outer part of the wave-function.
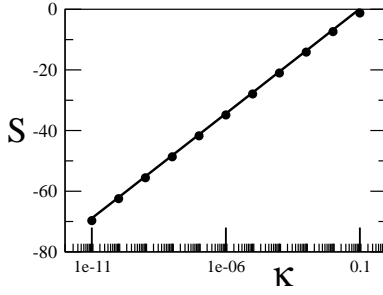

Fig. 3: Plot of S vs. $\ln \kappa$ with $a = 1$. The circles are the numerical values and the straight line is the predicted line $S = 3 \ln \kappa + 7.06$, Eq. 22.

To generalize the result for any dimension we carried out the calculation for general d. The density matrix, solely from the outer part, is expected to be of the form $f(\tilde{q}) \sim (1 + \tilde{q}^2)^{-2}$ as in previous cases but then there is a divergence problem for normalization for $d \geq 4$. Since we want $\text{Tr} \hat{\rho} = 1$, an ultraviolet cutoff is required. This makes $a\kappa$ an important variable even in the limit $a\kappa \to 0$. The specialty of $d = 4$ is now evident.

The radial wave function $R(r)$ ($l = 0$ state as the ground state) is,

$$R(r) = \begin{cases} A \ r^{\epsilon/2} J_{|\epsilon/2|}(kr) & \text{for} \quad r < a \\ B \ r^{\epsilon/2} H^{(1)}_{|\epsilon/2|}(i\kappa r) & \text{for} \quad r > a, \end{cases} \tag{23}$$

where $\epsilon = 2 - d$, A, B determine the normalization and matching of the inner and the outer solutions. Here J and $H^{(1)}$ are the Bessel and the Hankel function of the first kind. The continuity of the wave function at $r = a$ gives

$$A J_{\left|\frac{2-d}{2}\right|}(k_c) = B (\kappa a)^{-\left|\frac{2-d}{2}\right|}, \tag{24}$$

under the condition $\kappa \to 0$ and $ka \to k_c \to \pi/2$. Eq.3 follows from Eq.24, the matching of log derivative and the Bessel function identities. By using the normalization condition and Eq. 24, we get

$$B = \begin{cases} \frac{\bar{\kappa}}{a} & \text{for} \quad d < 4 \\ \frac{\bar{\kappa}^{|2-d|/2}}{a} & \text{for} \quad d > 4. \end{cases}$$

In the same $\kappa \to 0$ limit, with outer part dominance,

$$\phi(q = 0) \approx B\kappa^{-\frac{2+d}{2}}, \tag{25}$$

which gives

$$\hat{\rho}(\mathbf{q}) = |\phi(\mathbf{q})|^2 = B^2 \kappa^{-(2+d)} f(\tilde{\mathbf{q}})$$
$$\approx \begin{cases} \kappa^{-d} & \text{for} \quad d < 4 \\ \kappa^{-4} a^{d-4} & \text{for} \quad d > 4. \end{cases} \tag{26}$$

So the von Neumann entropy is of the form Eq. (15a) with $P = 4$ for $d > 4$.

In terms of the deviation from the critical point, the entropy is

$$S = \frac{d}{z(\Psi - 1)} \ln |u - u_c|, \quad \text{for } \Psi < 2. \tag{27}$$

For the case in hand, $\Psi = d/2$. The form of Eq. 27 brings out the universal behavior of the entropy and has validity for potentials different from Eq. 1, like e.g. scale-free $1/r^2$ potential [12]. All the details of the interaction go in the universal exponents z and Ψ. The entropy diverges at the critical point and, *is negative*.

DNA connection. – We show the connection of the quantum entanglement entropy to the entropy of bubbles in DNA melting. Under an imaginary time transformation, the path integral formulation of the quantum problem is analogous to a classical statistical mechanical system of polymers used in the context of melting of DNA [9–11, 14].

Let us consider a DNA whose two strands are two Gaussian polymers in d-dimensions and index the points (monomers) by the contour length z measured from one end. The native base pairing of a DNA requires that a monomer at index z on one strand interacts with a point on the other strand with the same index z. This is the Poland-Scheraga type model [11] for DNA melting. By using one extra coordinate for the sequence or the length of the polymers, we get directed polymers in $d + 1$ dimensions like paths in path integrals, as shown in Fig 2. In this representation the base pairing interaction maps onto the same time interaction of the quantum system, time playing the role of the base pair index. The DNA partition function as a sum over all polymer configurations is equivalent to the sum over all paths in quantum mechanics. The DNA Boltzmann factor $\exp(-\beta H)$ with β as the inverse temperature and H the Hamiltonian for two chains of elastic constants K_j as

$$\beta H = \int_0^N \left[\sum_{j=1,2} \frac{K_j}{2} \left(\frac{\partial \mathbf{r}_j(z)}{\partial z} \right)^2 + V(\mathbf{r}_1(z) - \mathbf{r}_2(z)) \right] dz, \tag{28}$$

corresponds to the factor $\exp(i\mathcal{S}/\hbar)$ for path integrals with $\mathcal{S}$ the classical action of two interacting particles under $z \to it$. This makes the Green function or the propagator

$\mathcal{G}(x_1, x_2, \tau | x'_1, x'_2, 0)$ equivalent to the partition function $Z(x_1, x_2, N | x'_1, x'_2, 0)$, $(N \to i\tau)$. Here x_j, x'_j are the coordinates of the j-th strand end-points at 0 and at length N. The free energy per unit length of DNA for $N \to \infty$ is the ground state energy of the quantum problem.

The short range base-pairing potential can be taken to be a contact potential or a well of Eq. (1). Then the picture of return of the quantum particles within the range of interaction after excursions outside the well gives the equivalent picture of polymers with broken base pairs having excursion away from binding and eventually coming back to the well to form pairs. This excursion swells the polymer and creates bubbles along the length of the DNA. Thermal energy opens up bubbles in the bound state of DNA. The entropy of a bubble of length N is determined by the reunion partition function of two polymers starting together and reuniting again at N, which for large N, has the form $\Omega(N) = N^{-\Psi} e^{N\sigma_0}$, or the entropy

$$S \equiv \ln \Omega(N) = N\sigma_0 - \Psi \ln N, \qquad (29)$$

in units of the Boltzmann constant $k_B = 1$. Eq. 29 shows that σ_0 is the bubble entropy per unit length that survives in the thermodynamic limit. However, the power law N-dependence which gives the negative sub-extensive part of the entropy is essential for the transition and also for the bound state. The reunion exponent Ψ determines the universality class of the binding-unbinding transition and there is a melting transition if and only if $\Psi > 1$. See Ref. [9] for details.

The one-dimensionality of the chains requires an alternating arrangement of bound regions and bubbles as in Fig. 2. The arrangement allows one to write the partition function, after Laplace transform with respect to the length (i.e. in the grand canonical ensemble) [9], as

$$\begin{aligned} G(x, y; s) &= G_o(x; s) G(0, s) G_o(y; s) \\ &= \frac{G_o(x; s) G_o(y; s) G^B(s, u)}{1 - G^U(s, \sigma_0) G^B(s, u)}. \end{aligned} \qquad (30)$$

Here $x \equiv \{x_1, x_2\}$, $y \equiv \{x'_1, x'_2\}$, G_o is the Laplace transformed partition function of two polymers tied at one end and open at the other, called the survival partition function, and $G(0, s)$ is the total partition function with two ends bound. In G_o, the tied point is to be integrated over keeping the set x or y fixed. $G(0, s)$ can be written as a sum of a geometrical series (see Fig. 2) involving the partition functions of the bound parts and the bubbles, $G^B(s, u)$ and $G^U(s, \sigma_0)$. The free energy comes from the singularity of $G(x, y, s)$ which is either $s = \sigma_0 \equiv 0$ or at $s = s_0$ for which

$$G^U(s, \sigma_0) G^B(s, u) = 1, \qquad (31)$$

with $\sigma_0 = 0$, s_0 satisfies Eq. (3).

Near the nontrivial singularity, a pole at $s = s_0$, the form of $G(x, y, s)$ resembles the Green function in the energy eigenfunction expansion as

$$\frac{\langle y | \psi \rangle \langle \psi | x \rangle}{E - E_0}, \qquad (32)$$

with ground state dominance. From the equivalence between DNA model and the quantum problem, we identify the density matrix as

$$\rho(x, y) \sim G_o(x; s_0) G_o(y; s_0) / G^U(s_0),$$

so that the entanglement entropy would behave like $S \sim \ln G^U(s_0, \sigma_0)$. By using Gaussian distributions for Gaussian polymers (i.e. random walkers), one recovers Eq. 21.

To get the behaviour of $\ln G^U$, we employ a finite-size scaling analysis. The phase transition in the polymeric system occurs in the $N \to \infty$ limit so that a finite N acts as a finite size scale both for DNA and in the quantum problem. The finite size scaling variable is $N/\xi_\perp^z$ so that the entanglement entropy is proportional to $-z \ln \xi_\perp \sim \frac{1}{\Psi-1} \ln | u - u_c |$ (see Eq. 27). The difference in the amplitude occurs because of the different normalization used for polymers and quantum problems. The point to note is that the entanglement entropy in the quantum problem comes from the universal non-extensive part of the entropy of the bubbles. Since the full entanglement spectrum is known, it is also possible to compute the Renyi entropy [6]. We recover in the appropriate limit the result quoted in Eq. 15a. In the DNA interpretation, the Renyi entropy would come from many circular single strands (replicas) pairing with a large single strand, resembling the rolling circle replication of viruses. Details will be discussed elsewhere.

Discussion. – A negative entropy is counter-intuitive when one has the third law of thermodynamics in the back of one's mind, though exceptions are known; e.g. negative entropy is found for perfect gases at low temperatures or as a corollary of the classical equipartition theorem. One can see the same feature by writing the reduced density matrix in terms of an entanglement Hamiltonian, $\rho \propto \exp(-\beta H_{ent})$, in a form reminiscent of a Boltzmann factor. The diagonal form in Eq. 21 shows

$$\beta H_{ent} = 2\ln(1 + q^2/\kappa^2) \approx 2q^2/\kappa^2, \text{ (for small } q), \quad (33)$$

which is like a classical d-dimensional oscillator in q-space, with κ^2 as the effective temperature. A direct calculation or use of the classical equipartition theorem now tells us that the entropy has $d \ln \kappa$ behaviour as in Eq. 15a. We believe this to be a generic feature whenever the entanglement Hamiltonian is gapless. Another way to see this emergence of $\ln \kappa$ in entropy is to compare with the DNA problem. The equivalent classical DNA model also has a negative diverging part of entropy but that sub-extensive part vanishes in the thermodynamic limit of the entropy per unit length. In the quantum case, the equivalent limit has no such advantage in finding the entropy because demanding extensivity in time direction is meaningless. Hence the negatively diverging term is inevitable near criticality.

In this paper we show that the quantum entanglement entropy near the bound-unbound transition of two inter-

acting particles comes out to be negative, and it diverges at the QCP. Using the equivalent classical statistical mechanical system of DNA near the melting transition we show that the negativity of the entanglement entropy is a necessity and is essential for the phase transition. The coefficient of the logarithmic term contains the information of the interaction and the universal behaviour of the phase transition. The coefficient is shown to be related to the reunion exponent of vicious walkers. This is the first time in the context of quantum entanglement that the negative entropy is found by explicit calculation. We argue that this log divergence in the quantum case and the sub-extensive part in the DNA problem are linked by finite size scaling near the critical point. From the renormalization group (RG) approach for the DNA melting problem [10,12], one may infer that the entanglement entropy increases along the RG flow, since the critical point corresponds to the unstable fixed point. It has been argued recently that entanglement can be used to produce negative entropy [15]. The information theoretical meaning of the negative entropy in our case is not very clear. Our speculation is that the negative entropy is the norm, not an exception near a quantum binding-unbinding transition. We feel signatures of negative entropy might be detectable in cold atoms where interactions can be tuned to the unitarity limit. If one can harness the negative entropy, one may cool a system or a computer and possibly may overcome the obstacle to circuit miniaturization.

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